Modeling the Thermal Response of Explosives

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Objective

- Predict the response of HE
  - STS
    - What is the state of the HE upon delivery?
  - Abnormal
    - What is the state of the HE after an abnormal event?
    - Will the HE release energy?
      - If so, how much?

HE Response

- Detonation
  - *“reactive-wave phenomena whose propagation is controlled by shock waves”*
    - “Numerically Modeling of Explosives and Propellants,” Charles Mader
- Thermal Response
  - Energy release but no shock wave
  - Energy *can* approach that of a detonation
  - a.k.a. Non-Shock initiation

Thermal Response

- Caused by temperature increase
  - Mechanical loading
    - adiabatic heating
    - viscous dissipation
    - pore collapse
    - friction
    - cracking work
  - External temperature increase

Thermal Response

- Chemical decomp. = energetic release
  - Modeling question:
    - How does the mechanical and thermal loading combine with the chemical decomposition to produce energy?
  - Possible answers:
    - Self sustaining reaction - Initiation
    - Quenched reaction - small energy release
    - No reaction

Thermal Response Scenarios

- Usually unintended accident scenarios
  - Abnormal Heat Environments
    - Processing fires
    - Transportation accidents
  - Abnormal Mechanical Events
    - Handling accidents
    - Transportation accidents
    - Hostile attacks

Modeling

- Determine
  - Will the HE react?
  - If it does, how violent is the reaction?
- The model must
  - predict the structural response of the HE
  - determine the interaction between the mechanical/thermal loading and chemical decomposition

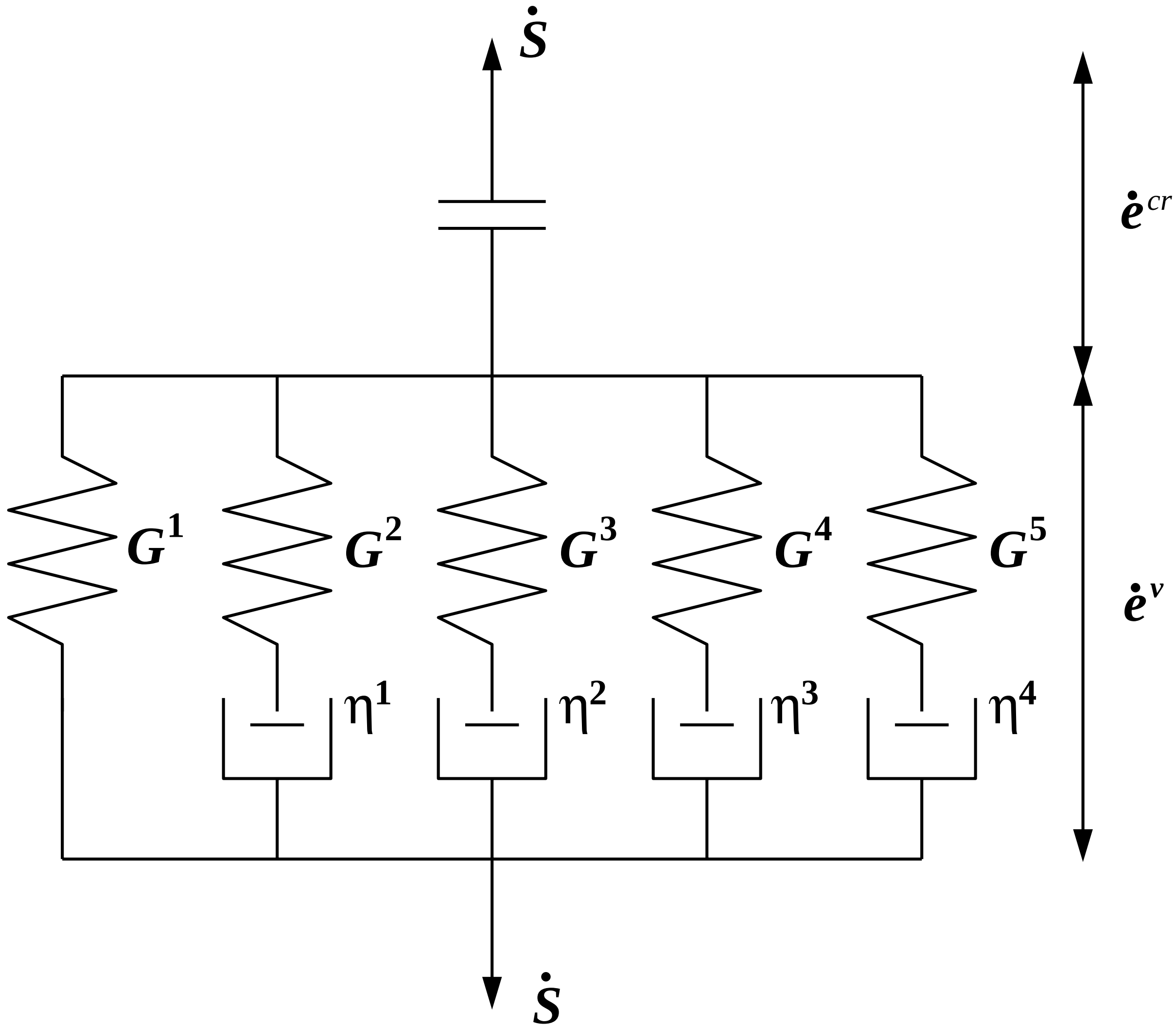
PBX Response

- Brittle HE particles bonded with polymer
  - Mechanical
    - Composition suggests a rate dependent material that will lose strength as load is applied (i.e. a visco-elastic damage model)
  - Thermal
    - Primarily governed by HE particles
      - mechanical work done on particle causes temperature increase and chemical decomposition
- Continuum Model - ViscoSCRAM
- Discrete Cracking

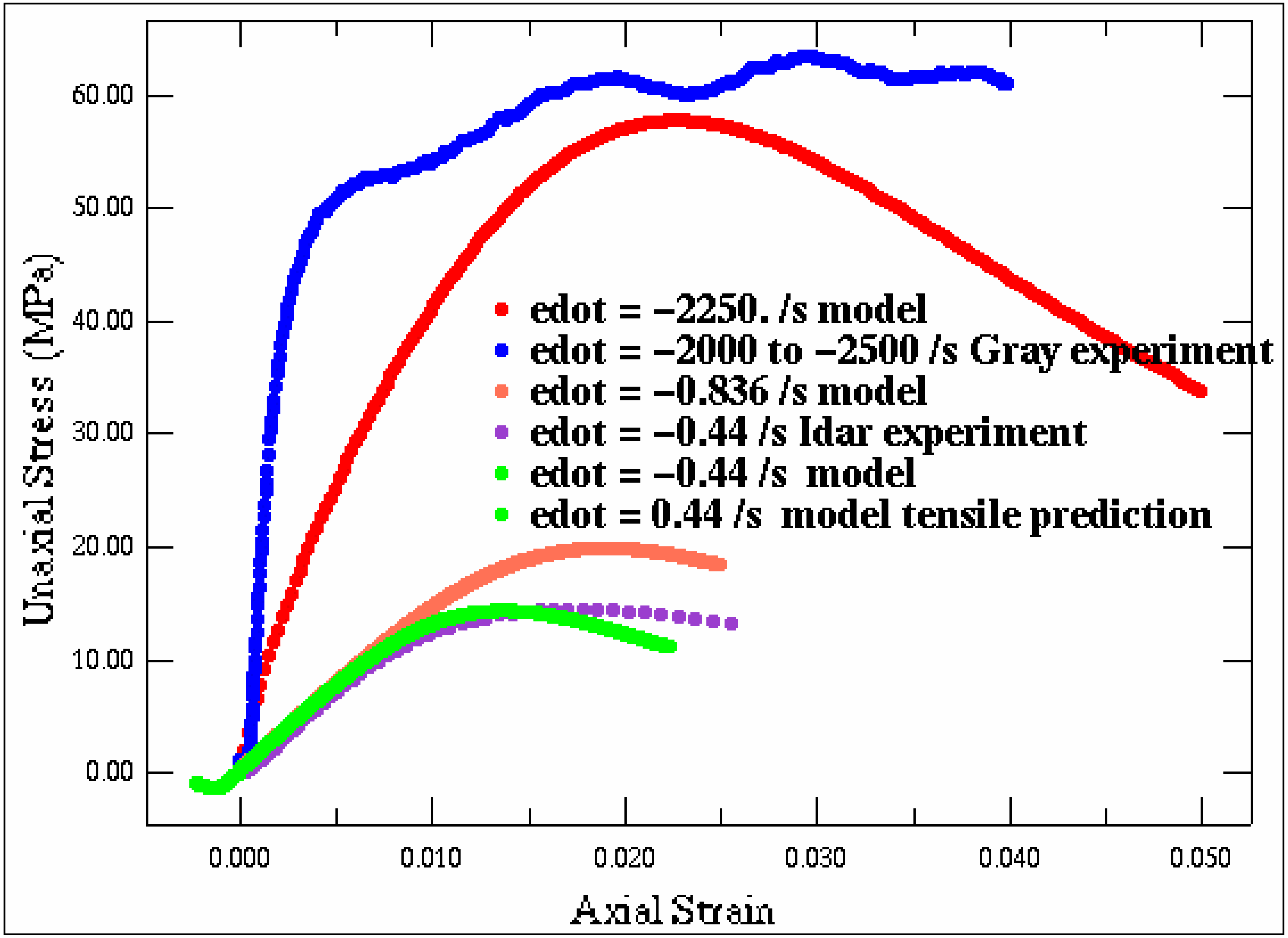
Mechanical Response - ViscoSCRAM

- Visco - Elastic
  - Isotropic, Generalized Maxwell Model
- Continuum Damage
  - Statistical Crack Mechanics (SCRAM)
    - Statistical Dist. of Randomly Oriented Micro Cracks
    - Rate Dependant Crack Growth
    - Crack Face Friction

ViscoSCRAM - Mechanical



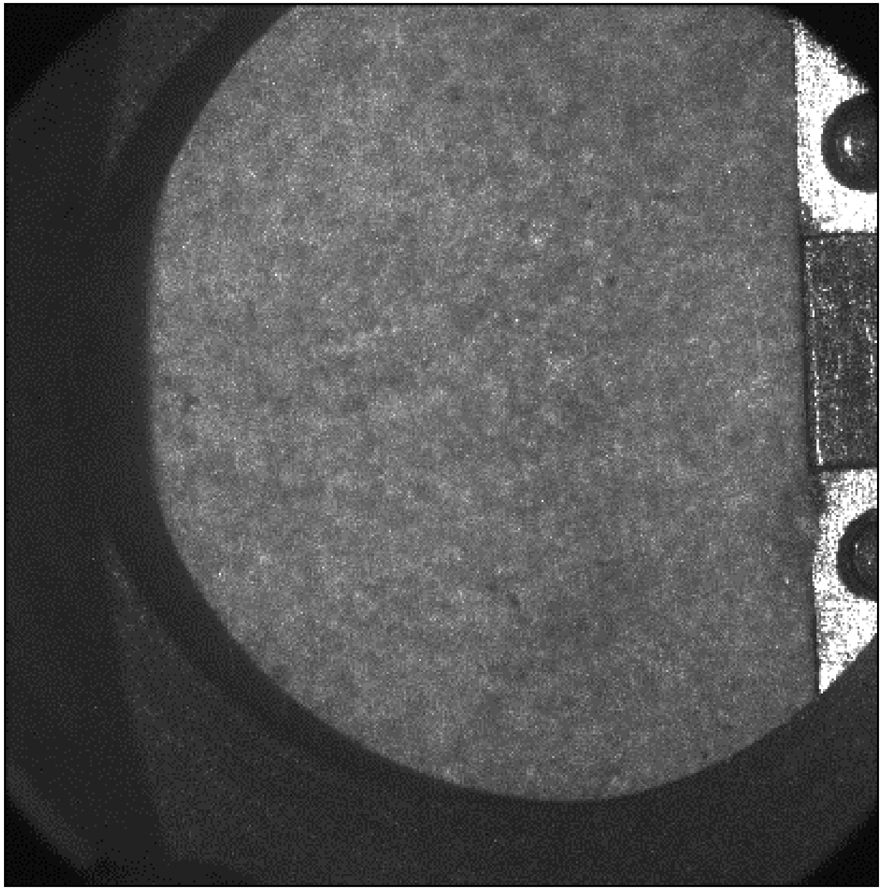
ViscoSCRAM - Mechanical

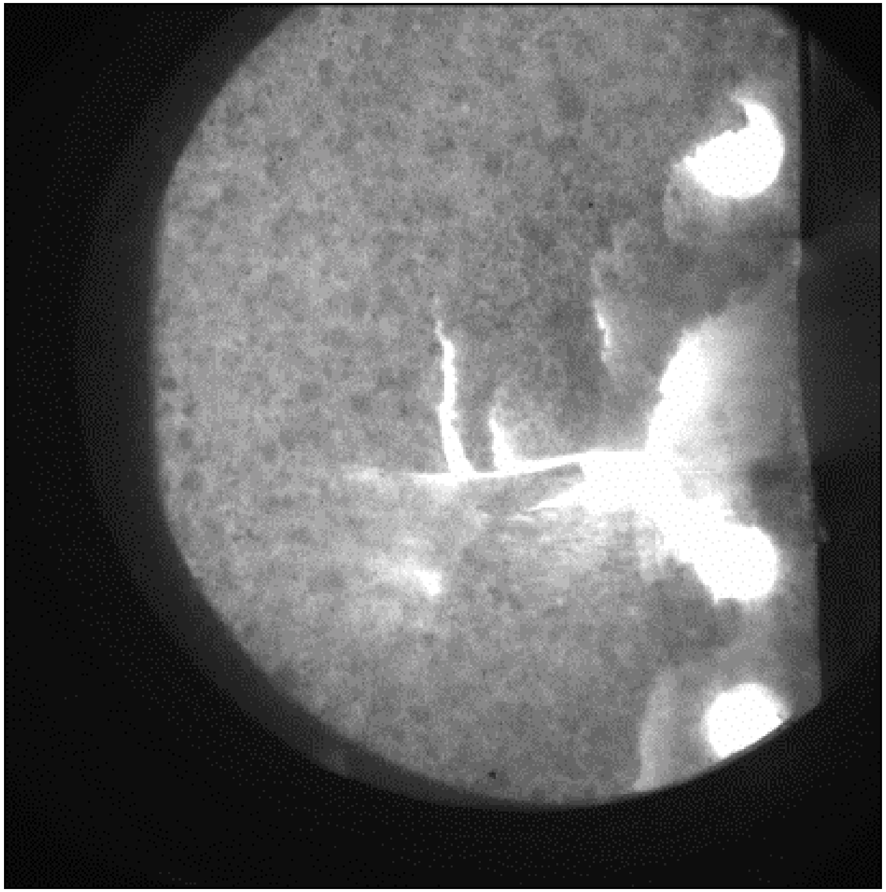


Mechanical Response - Discrete Cracking

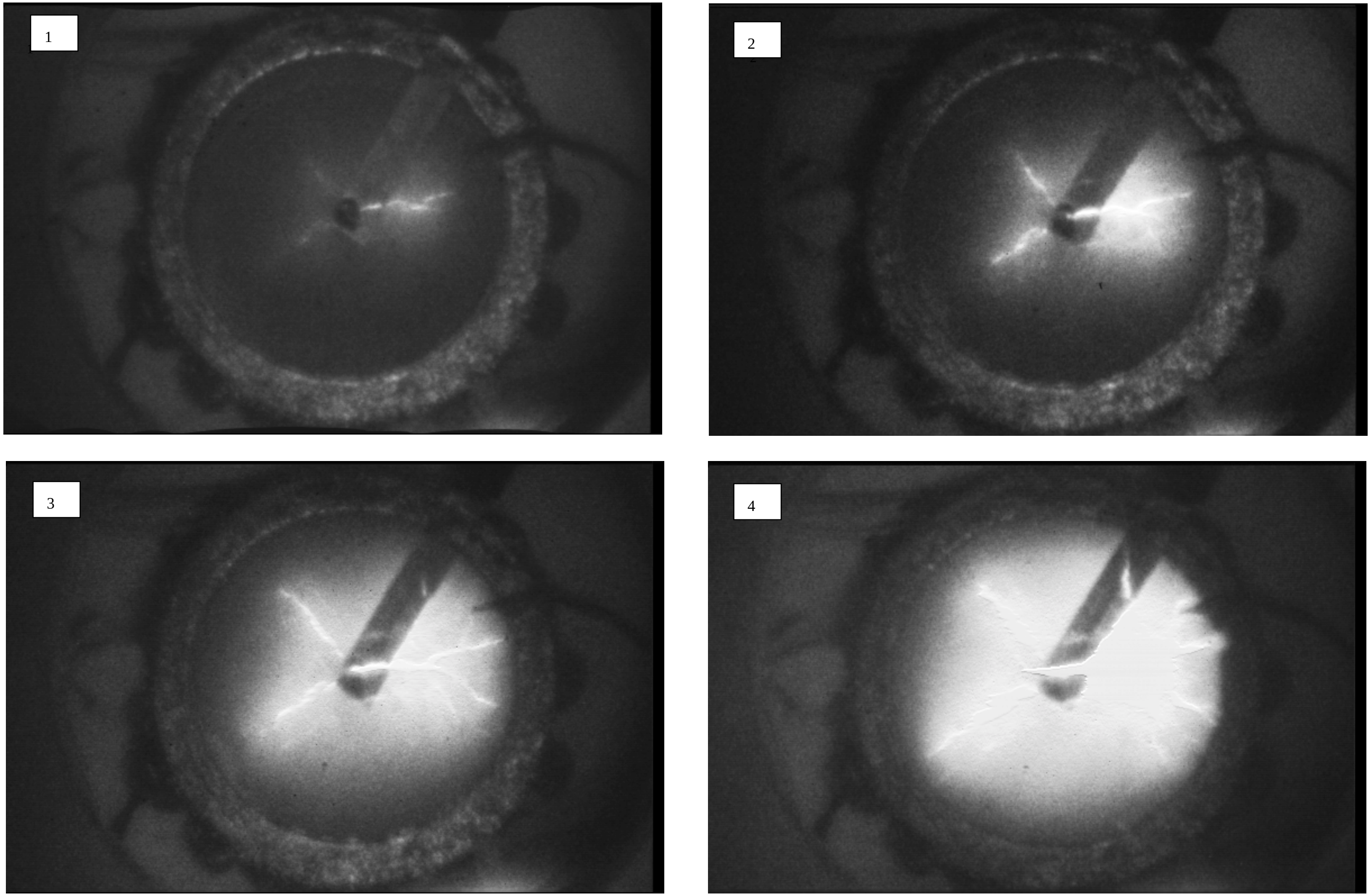
- Large Macroscopic Cracks
  - Change material response
  - Change geometry
  - Can increase reaction violence
    - Exposed surface is easier to burn
    - Release of decomposition gases
      - Ignition causes additional mechanical/thermal load

Mechanical Response - Discrete Cracking





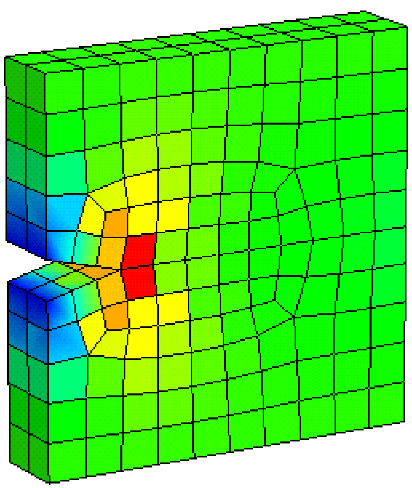
Mechanical Response - Discrete Cracking



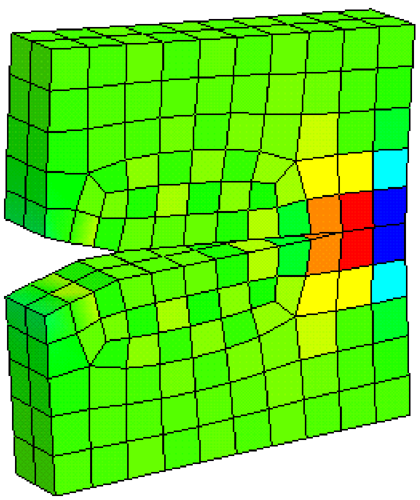
Mechanical Response - Discrete Cracking

- Method:
  - ⇒ Standard FE Model
  - ⇒ Bond Elements Together
  - ⇒ Evaluate Failure Criteria @ Each Interface
  - ⇒ Release Bond for Fracture

Standard "Bonded" FE Model



Bond Released Along Fracture



Failure Criteria

- Failure Based on Stresses from Adjacent Elements
  - Stress @ interface - $\bar{\sigma} = \frac{\sigma_1+\sigma_2}{2} \quad \bar{\tau} = \frac{\tau_1+\tau_2}{2}$
- Failure Criteria
  - Interface Normal Stress

$$\bar{\sigma}_n \geq \sigma_f$$

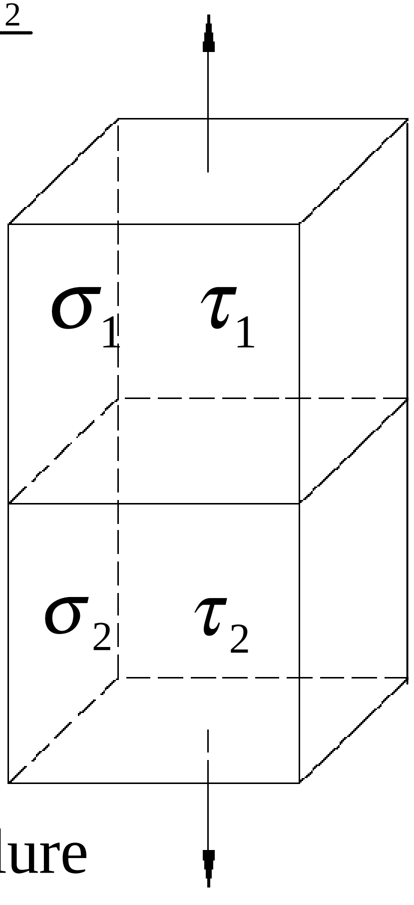
  - Effective Stress

$$|\sigma| \geq \sigma_f$$

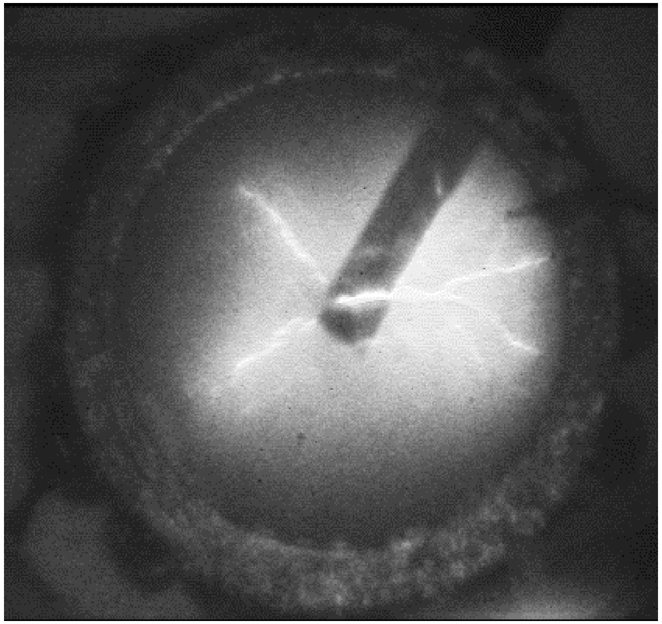
  - Fracture Energy

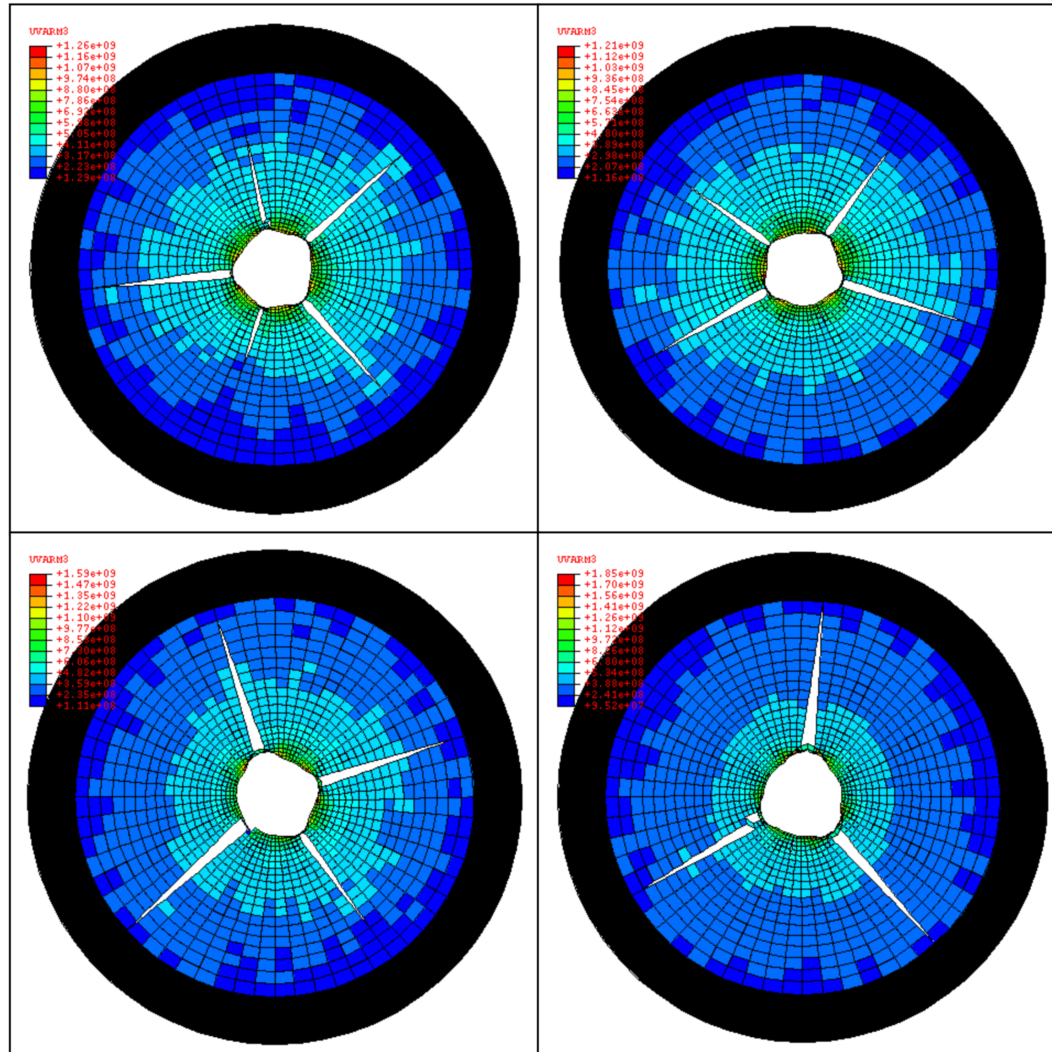
$$K_I = \bar{\sigma}\sqrt{\pi \cdot a} \qquad K_{II} = \bar{\tau}\sqrt{\pi \cdot a}$$

  - Stress Bridging (HE Model)
    - Resistive Forces @ Interface after Failure



Mechanical Response - Discrete Cracking





Using randomized failure criteria, the simulations show qualitative agreement with experimental results

Thermal - ViscoSCRAM

- Bulk Heating
  - Mechanical
    - Viscous
    - Cracking
    - Adiabatic Volume Change
  - Chemical Decomposition
    - Arrennius First Order Chemical Kinetics
- Hot Spot Heating
  - Crack face friction

ViscoSCRAM - Bulk Heating

$$\dot{T} = \alpha T_{,ii} - \gamma T \dot{\varepsilon}_{jj} + \frac{\Im}{\rho C_v}\left[(\dot{w})_{ve} + (\dot{w})_{cr}\right] + P_{he}\dot{q}_{ch}$$

$\boxed{\alpha T_{,ii}}$ – Rate of conduction

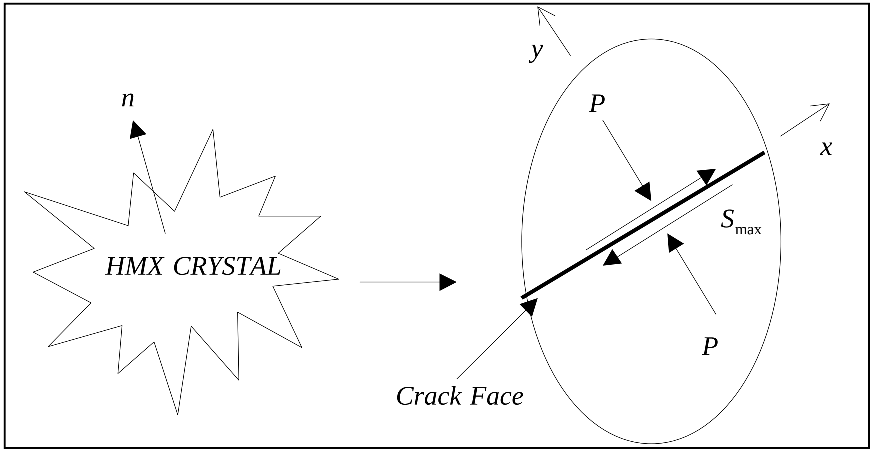
$\boxed{\gamma T \dot{\varepsilon}_{jj}}$ – Adiabatic compression heating rate

$\boxed{\frac{\Im}{\rho C_v}(\dot{w})_{ve}}$ – Visco-elastic work rate

$\boxed{\frac{\Im}{\rho C_v}(\dot{w})_{cr}}$ – Cracking work rate

$\boxed{P_{he}\dot{q}_{ch}}$ – Bulk chemical heating rate

ViscoSCRAM - Hot Spot



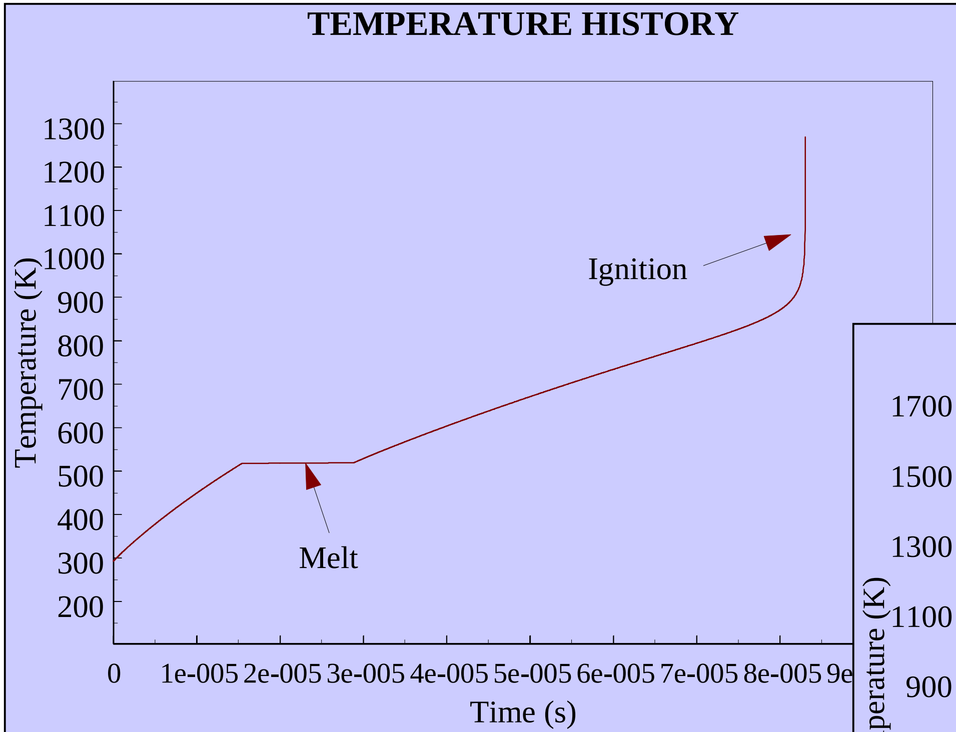
$$\rho_f C_f \dot{T} = \frac{\partial}{\partial y}\left(k_f \frac{\partial T}{\partial y}\right) + \rho_f \Delta H Z e^{-E/RT} - \mu_d \sigma_m \frac{\partial v_x}{\partial y}$$

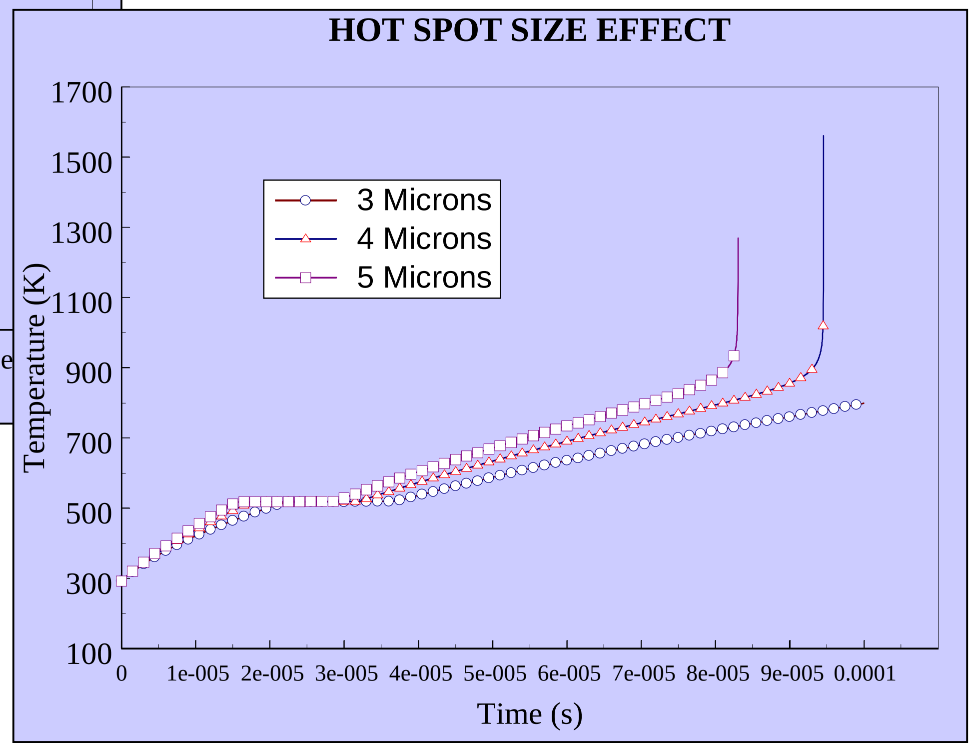
$$l_f \geq y \geq 0$$

$$\rho_s C_s \dot{T} = \frac{\partial}{\partial y}\left(k_s \frac{\partial T}{\partial y}\right) + \rho_s \Delta H Z e^{-E/RT}$$

$$y > l_f$$

ViscoSCRAM - Thermal





Status of Thermal Modeling

- ViscoSCRAM ignition is being calibrated/validated
  - “Tuning” parameters in the model to match experimental results
    - SS HEVR
    - Stevens
    - Asay Impact
  - Simple experimental results are limited

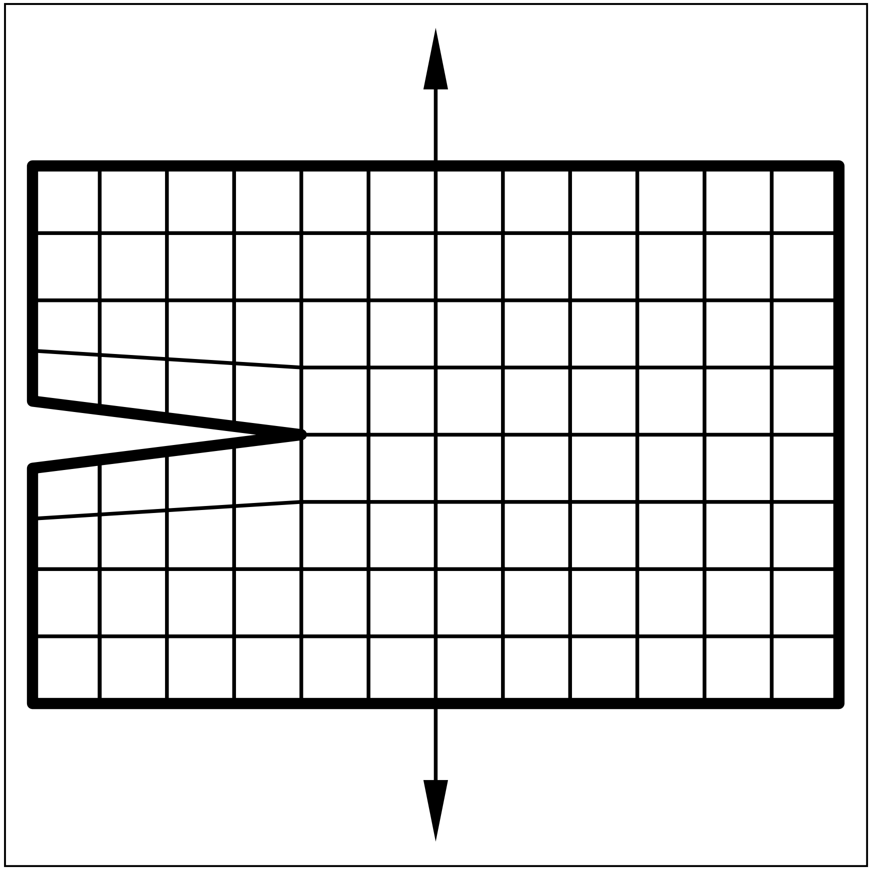
Future of Thermal Modeling

- To capture reaction violence, a model for discrete cracking, gas evolution and ignition must be developed
  - The concept:
    - Models for gas evolution exist
    - Discrete Crack model predicts cracking
    - All that is left is to couple the two models
  - The implementation may not be simple

Burning Cracks

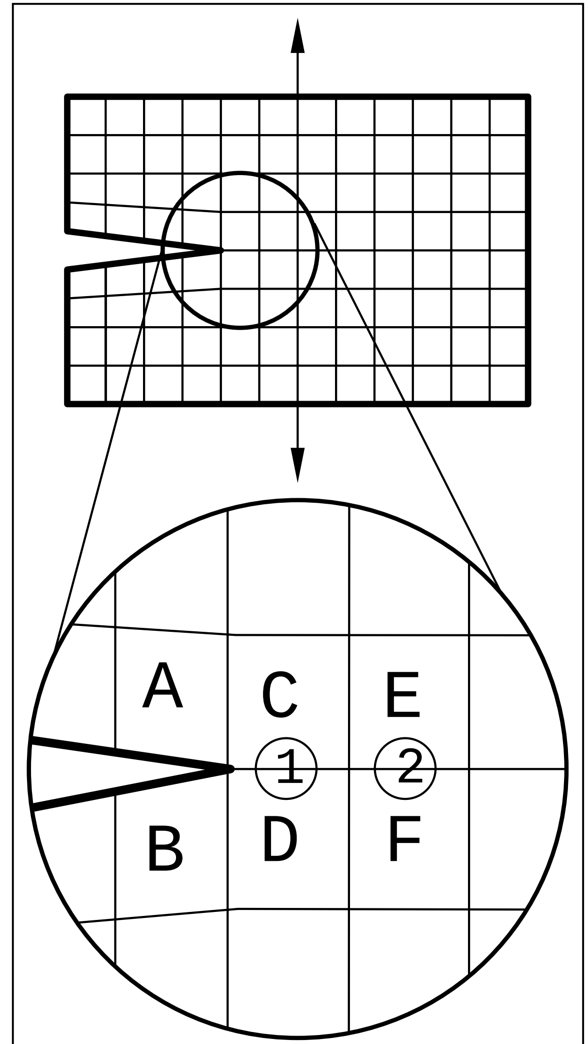
Abstract Concept:

- → Gas in crack
- → Gas may ignite
- → Load crack faces
- → Crack accelerates
- → Transports reaction



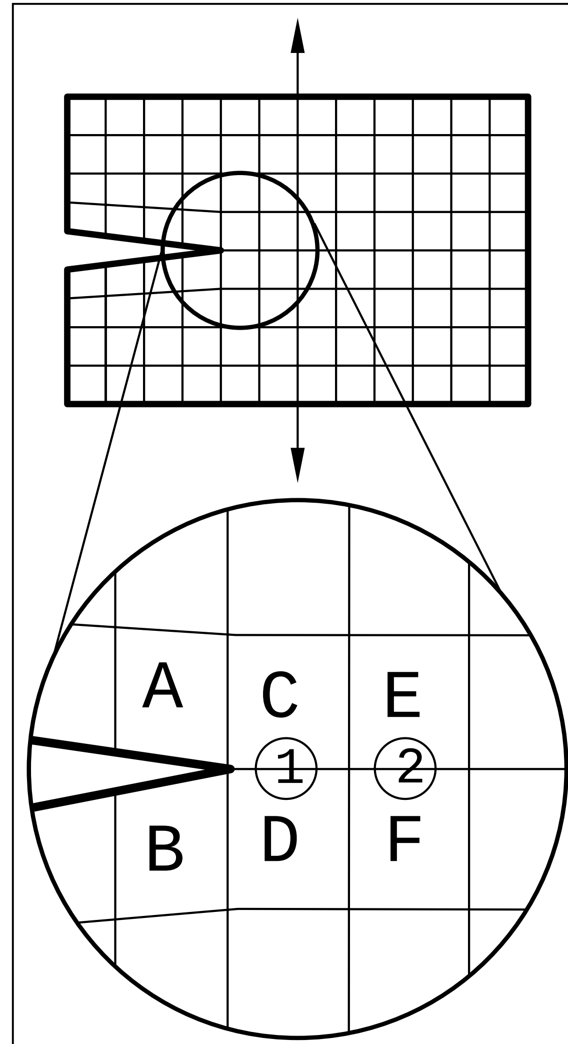
Burning Cracks

- Modeling - 1st cut
  - Structural/Thermal loading
    - Gas evolution in HE
    - Increased Stress @ Crack Tip
  - Interface 1 breaks
    - 2D surface is now a volume
  - Gas escapes from C & D to adjacent volume
  - Ignition causes pressure
  - Increased load on C & D
  - Interface 2 breaks
  - Cycle continues



Burning Cracks

- Difficulty - The process is global
  - Gas in cavity 1 is not only from C & D
  - Ignition is dependent on whole crack geometry
  - Ignition/Flame propagation is a function of pressure



Burning Cracks

- Currently a conceptual model
- Timeframe for implementation is unknown

Conclusions

- Thermal Response of HE requires both mechanical and thermal models
  - Structural response - determines the bulk and hotspot thermal response
  - Crack model - determine the extent of reaction and reaction violence
- Calibration of ignition model is ongoing
  - Provides the best answer to “Will the HE release energy?”
  - Does not answer “How much energy?”